Ethyl ethylcarbamate
623-78-9 | DTXSID0060775

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.95	0.69	0.95	0.65	0.96	0.68

Model Results

Predicted value: 4.91

Global applicability domain: Inside

Local applicability domain index: 8.56e-01

Confidence level: 5.88e-01

Nearest Neighbors from the Training Set

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Cyclohexanol
Measured: 5.18
Predicted: 4.72

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1-Hexanol
Measured: 5.18
Predicted: 4.67

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1-Octanol
Measured: 6.03
Predicted: 5.95

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Dipropylamine
Measured: 3.59
Predicted: 4.37

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Piperidine
Measured: 4.04
Predicted: 4.32